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東京大学理学部 1 号館西棟 11 階 1109 号室 (天文学専攻会議室) にて

“Surface chemistry in astrochemical models”

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With the advent of the new generation of mm and sub-mm detectors (ALMA, NOEMA), molecules are detected in a large variety of galactic and extra-galactic interstellar environments. These molecules are unique probes to investigate the physical and chemical processes in interstellar gas and on grains. State-of-the-art astrochemical models have to take into account consistently both gas phase and surface chemistry to interpret observations and, to do so, they must rely on theoretical and laboratory experiments results. However, surface chemistry is complex to implement in astrophysical codes, in which grain models are necessarily simplified.

We have implemented surface chemistry for H, C, and O bearers in a new version of the Meudon PDR code, one of the state-of-the-art public astrochemical code (<http://ism.obspm.fr>). In particular, H<sub>2</sub> formation on grains is a complex process, highly dependent on grain temperature. Small grains, the largest contributors, undergo temperature fluctuations caused by the absorption of UV photons. These fluctuations can significantly affect surface processes, such as H<sub>2</sub> formation or ortho/para conversion of H<sub>2</sub>. We have thus developed several formalisms to simulate H<sub>2</sub> formation mechanisms on grains in the Meudon PDR code. In particular, I have developed a new statistical formalism based on a master equation approach to compute the average efficiency of surface processes perturbed by fluctuations of the grain temperature.

In this talk, I will first demonstrate the critical influence of H<sub>2</sub> formation on emission lines in PDR, and in particular show that the high-J CO ladders observed by Herschel are signatures of high H<sub>2</sub> formation efficiency at the edge of PDRs. I will discuss how this efficiency can be explained by the Eley-Rideal mechanism. I will then present a new stochastic formalism for surface processes with dust temperature fluctuations, and demonstrate its application to both H<sub>2</sub> formation and ortho-para conversion of H<sub>2</sub> on grains, in relation to observations of H<sub>2</sub> rotational emission in PDRs. I will finally discuss how the relation between H<sub>3</sub><sup>+</sup> abundance and the cosmic ray ionization rate in the Galactic Center is highly dependant on H<sub>2</sub> formation efficiency. If time allows, I will also present the modelling of C and O surface chemistry in the Meudon PDR code, in relation to observations of organic molecules such as methanol in the Horsehead nebula.